BRIEFING on
PROGRAM SOLICITATION NSF05-570

Dynamic Data Driven Application Systems (DDDAS)

A new paradigm for
applications/simulations and measurement methodologies

Sponsored by NSF, NIH, NOAA
Cooperating Programs:
EU Grids & e-Infrastructure, and UK e-Sciences
Solicitation announced on March 10, 2005
Proposals due: June 13, 2005

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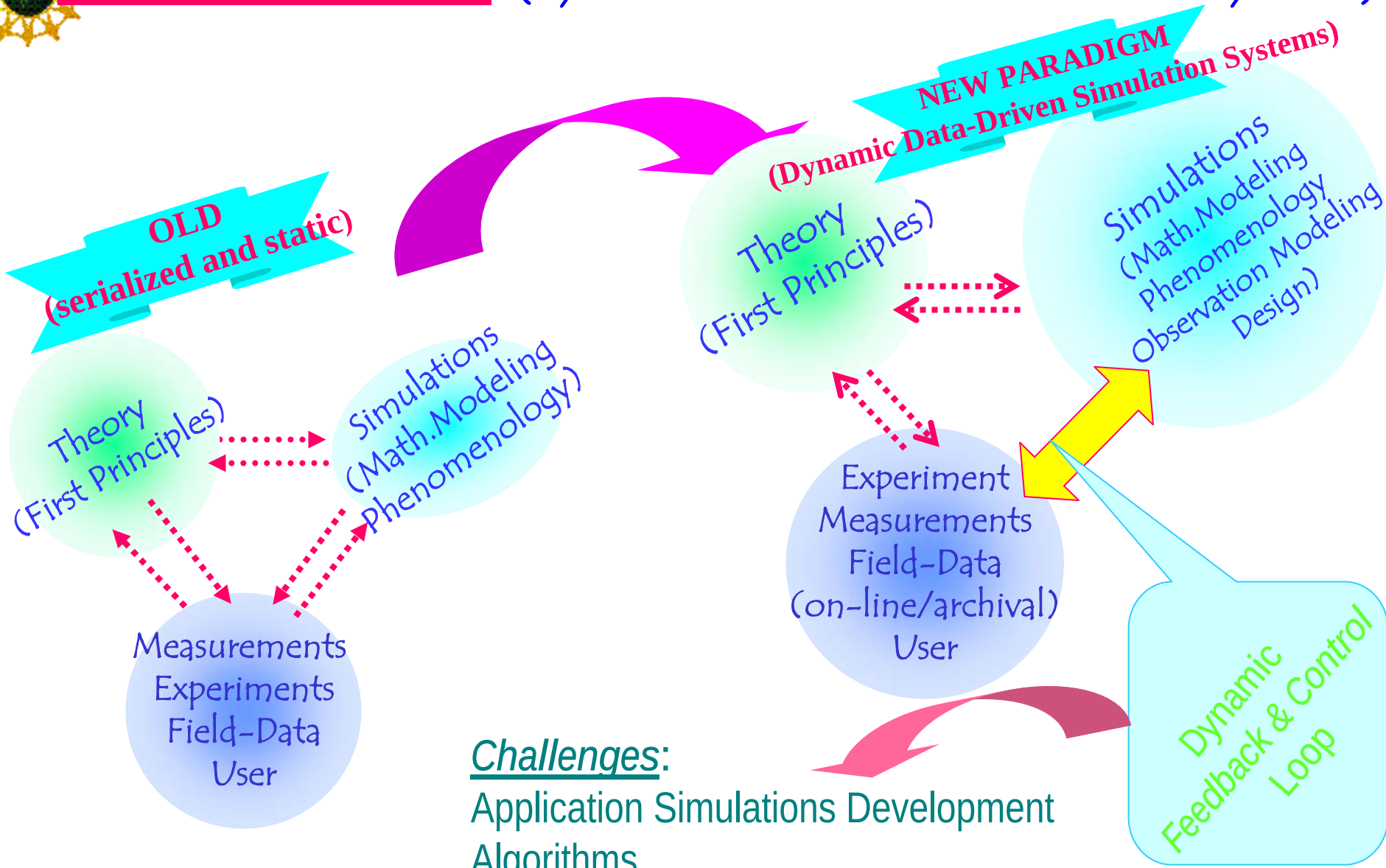
OUTLINE of BRIEFING

- Overview of the DDDAS concept
- Sponsors of this Program Solicitation
- DDDAS Program Description:
  - Research and Education Themes
  - Specific Emphasis Aspects of some sponsors
  - Award Information
- Cognizant Program Officials
- Summary

What is DDDAS (Symbiotic Measurement&Simulation Systems)



Challenges:

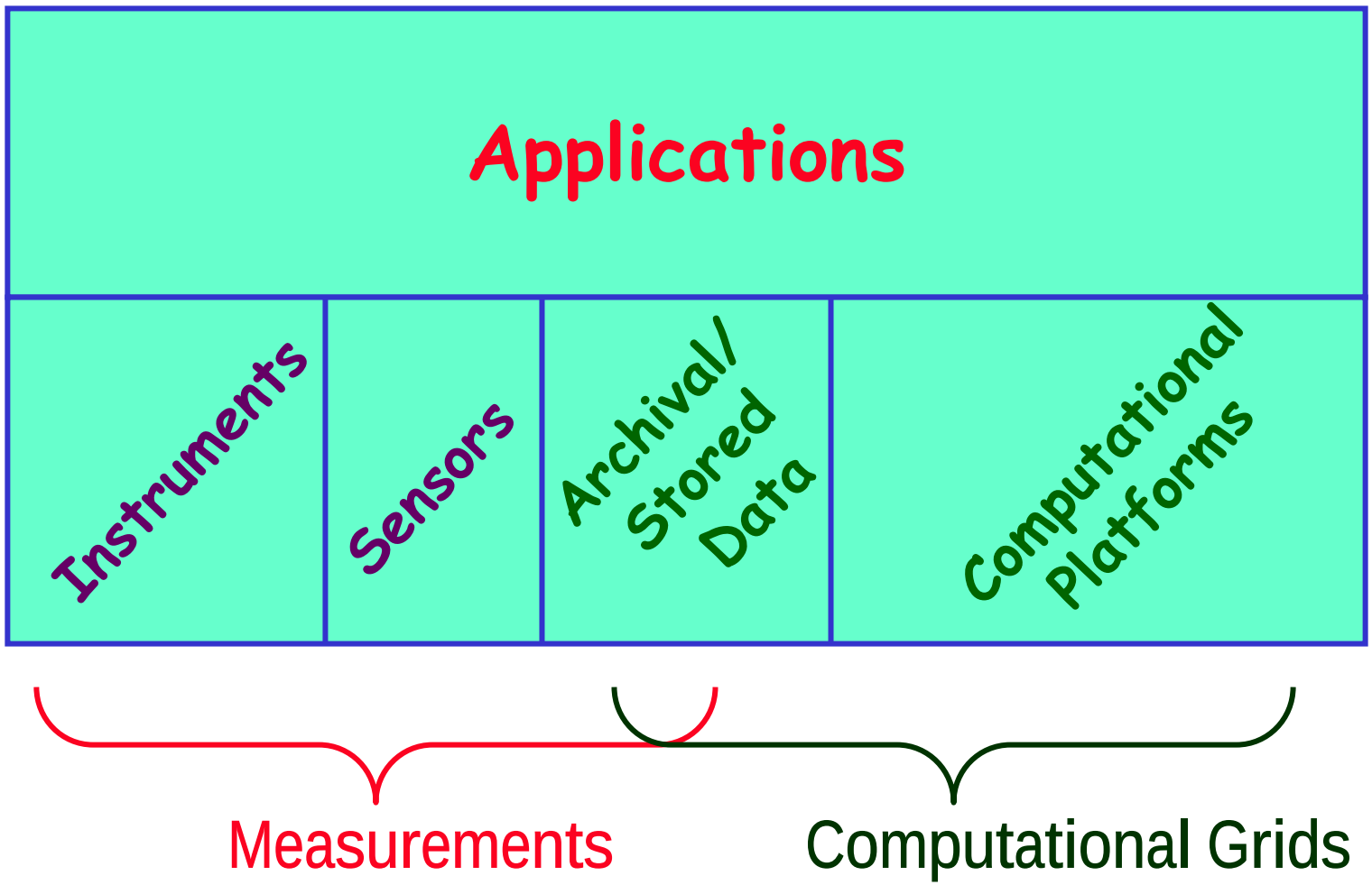
Application Simulations Development

Algorithms

Measurement Instruments Interfaces

Computing Systems Support

Beyond Grid Computing
"Extended Grid":
the Application Platform is
the computational&measurement system



Examples of Applications benefiting from the new paradigm

- Engineering (Design and Control)
  - vehicle/aircraft design, oil exploration, semiconductor mfg, structural eng, …
  - Computing systems hardware and software design and runtime
- Crisis Management and Environmental Systems
  - transportation systems (planning, accident response), …
  - weather, hurricanes/tornadoes, floods/tsunamis, fire propagation, pollution studies, …
- Medical
  - Imaging, customized surgery, radiation treatment, …
  - BioMechanics /BioEngineering, …
- Manufacturing/Business/Finance
  - Supply Chain (Production Planning and Control), …
  - Financial Trading (Stock Mkt, Portfolio Analysis), …

…MANY MORE EXAMPLES ARE LISTED
IN THE DDDAS PPROGRAM SOLICITATION
and the DDDAS webpage: www.cise.nsf.gov/dddas

NSF, NIH, NOAA Participants

- **National Science Foundation**
  - Directorate for Computer and Information Science and Engineering
  - Directorate for Engineering
  - Directorate for Education and Human Resources
  - Directorate for Mathematical and Physical Sciences
  - Directorate for Social, Behavioral, and Economic Sciences
  - Office of International Science and Engineering
  - Industrial Innovation Programs (SBIR/STTR)
- **National Institutes of Health**
  - National Institute of General Medical Sciences
  - National Library of Medicine
- **National Oceanic and Atmospheric Administration**
  - High Performance Computing and Communications Office

International Collaborations

Cooperating International Programs

- **EU Information Society Technologies (IST) Programme**
  - **EU e-Infrastructure**
  - **EU Grid Research**
- RCUK: Research Councils UK
  - **UK e-Science Program**

In addition:

The DDDAS Program Solicitation encourages international collaborations in accordance with the portfolio of activities and scope of countries of the NSF Office of International Science and Engineering

Industrial Collaborations

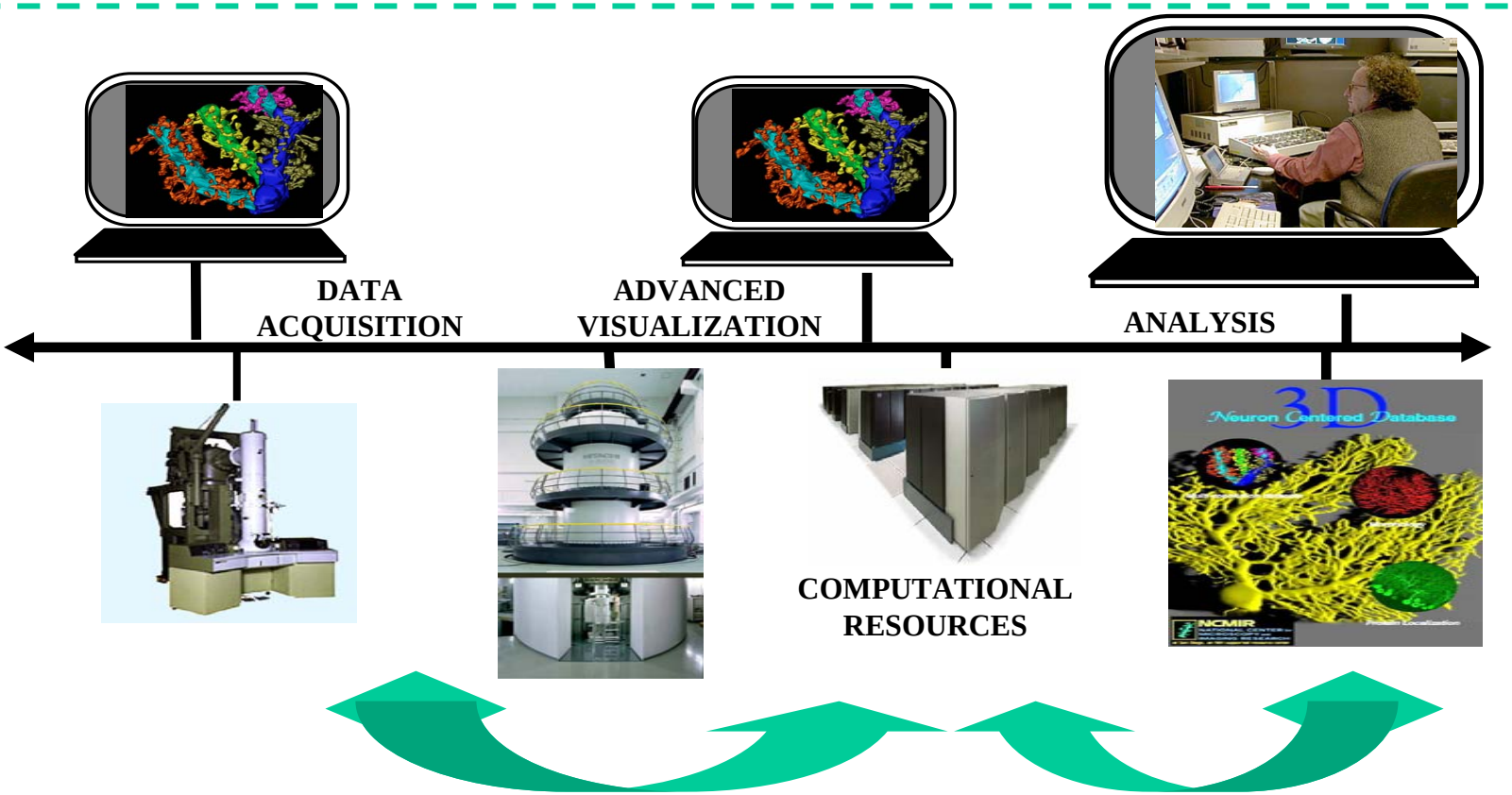
- The participation of the
  - NSF SBIR/STTR Program
  - EU and UK programs

  encourage collaborations with industry
- Proposals including industrial collaboration:
  - must include specifics on the role of the industrial partner and technical contributions to the project
  - means of funding the industrial partner
    - predominant funding venue for the industrial partner, will be via separate submission by the industrial collaborator to the above referenced programs as specified in the solicitation
    - in limited cases via subcontract to a funded project

- CLARIFICATION: NOT ALL PROPOSALS SUBMITTED TO THIS SOLICITATION NEED TO HAVE AN INDUSTRIAL PARTNER

DDDAS: Beyond Grid Computing

New Capabilities in Applications and Measurements



Some Technology Advances to Enable DDDAS

- **Application development**
  - multi-modal, multi-resolution application models
  - ability to dynamically switch to appropriate algorithms/components depending on streamed data
  - interfaces of applications with measurement systems
- **Mathematical and Statistical Algorithms**
  - tolerant to perturbations from dynamically input data
  - handling data uncertainties
- **Systems Software supporting such dynamic environments**
  - dynamic execution support on heterogeneous environments
  - extended spectrum of platforms: assemblies of Computational Grid platforms, Sensor Networks and Measurement Systems
- **Measurement Systems**
  - observational systems interfaced and steered by application requirements to optimize data collection at operational cycle
  - data-format, time-scale, sampling rate correlation of measurement systems under application-driven control

Research and Education Themes

- Developing DDDAS capabilities requires synergistic multidisciplinary research projects spanning in a balanced way:
  - Applications Modeling Methods
  - Mathematical and Statistical Algorithms
  - Systems Software Methods and Infrastructure
  - Measurement Systems and Methods
- Research advances in projects must:
  - either enable a DDDAS application (together with commensurate research advances in all four areas above)
  - or, advances in math&stat algorithms, systems software or measurement methods, must be driven by a specific DDDAS application
- Projects intending to have significant focus on measurement and instruments development, or infrastructure for such systems must comply with guidelines in the "agencies' specifics" section

Applications Advances

- Application steered by dynamic data inputs and application control of measurement processes
- Examples of capabilities to be developed:
  - application models describing system in different levels of detail and different modalities, and dynamic invocation of such models depending on dynamically injected data
  - Incorporating in application models asynchronously collected data, and combining data (measured, computed, archival) taken at different spatial or temporal scales
  - Dynamic application composition, dynamic selection of application models depending on dynamically injected data
  - Application-Measurement interfaces and data models, application-measurement time scale correlation
- + additional info in solicitation…

Mathematical and Statistical Algorithms Advances

- Algorithms stable under perturbations from dynamic inputs
  - numeric and stochastic algorithms
  - enhanced estimation and prediction algorithms
  - adaptive asynchronous algorithms
  - dynamic meshing, "patched meshing", and varying discretization schemes depending on dynamic inputs
  - continual optimization and stochastic methods to adaptively incorporate sampled data into the algorithm
- Handling uncertainty
  - methods to assess the quality of measurement errors and define the error bars of the dynamic inputs in reference to the initial or other static inputs
  - fast methods estimating propagation of measurement errors and impact to the fidelity and error bounds of the results of the uncertainty of dynamic inputs
- + additional info in solicitation…

Systems Software Infrastructure

- Dynamic Application Execution Support:
  - Systems Software to support dynamic composition of applications, like knowledge-based repositories and advanced compiler technologies to automate selection of application components
  - dynamic resource discovery and optimized mapping of applications as their computational requirements change depending on the injected data
- Interfaces to distributed physical devises and dynamic data management:
  - Management of measurement systems, sensor networks, etc, that augment the computational aspects of the applications platforms
  - Modeling of networked computer and sensor network resources, and measurement systems to support fault tolerance and quality of service for DDDAS environments
- + additional info in solicitation…

Measurement Systems

- Improvements in measurement, observation, and instrumentation methods, both at the design and operation cycle of measurement instruments
- Interfaces to such systems so that the executing application can control the measurement process and target the kinds of measurements to be collected
- Improvements in the means and methods of collecting data, such as focusing in the region of relevant measurements, more efficient sampling rates, power management of sensor systems, and determining the architecture of the sensor systems and networks transporting the data streamed into an executing application
- + additional info in solicitation…

Agencies' Specifics

- While the overall scope of the solicitation is broad in terms of the kinds of applications of interest, and the research projects to be supported should have a synergistic and balanced mix of the four areas discussed in the solicitation,

  Some of the sponsors of this solicitation place emphasis in specific application areas, or more emphasis in the development of observational instruments and systems;

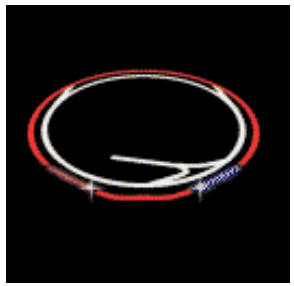
  These emphasis areas are stated in subsections in the "Agencies' Specifics" section in the solicitation
- For example,
  - for the NSF MPS Directorate, in addition to the broader interests, there is emphasis on measurement and instruments, and infrastructure to support such instruments, as stated under the NSF/MPS subsection
  - For NIH and NOAA, in the respective subsections the sponsors certain application areas
- Proposals that might be candidates to be co-funded by more than one sponsoring entity must satisfy the specific interests of such potential sponsors
- Proposers are encouraged to discuss such aspects with congnizant officials listed in the solicitation and the dddas webpage

EXAMPLE OF OBSERVATION SYSTEMS OF INTEREST TO NSF/MPS

ACCELERATOR APPLICATIONS OF DDDAS

Real time (local) control of charged particle accelerator systems: Accelerators now in design for many uses from bioscience to nanotechnology have very demanding requirements such as holding beams on target with accuracies of microns or even nanometers. Achieving this requires extremely precise control of hundreds of parameters.

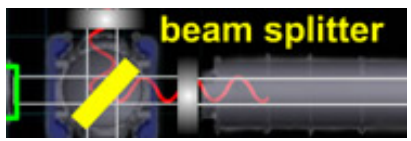
Global Accelerator Network GAN

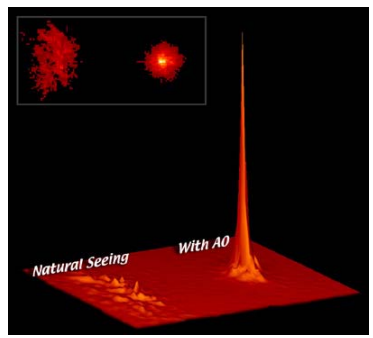


- **International Collaboration on Accelerator**
- **Far remote Operation**
- **Technical Issues**
- **Networking Issues**

SIMILAR CONSIDERATIONS HOLD FOR OTHER LARGE SCIENTIFIC FACILITIES

- *** Control Systems Within Facility**
- *** Remote Operation of Facility**
- *** SNS, SDSS, LIGO, ERL....**





Astronomical Adaptive Optics

- Adaptive correction of aberrations introduced by the Earth's turbulent atmosphere can allow ground-based optical/infrared telescopes to work at their *diffraction limit,* thereby achieving resolution better than space-based instruments.
- Next generation adaptive optics systems will require:
  - Sensing of the wavefront errors with very fast cameras
  - Modeling of the atmosphere's turbulent structure (tomography)
  - Commanding several deformable mirrors with thousands of degrees of freedom
- Atmospheric coherence time is of order milliseconds so the adaptive optics measurement-analysis-correction loop must run at kilohertz rates.
- Areas under development include: high speed sensors, atmospheric reconstruction algorithms, developments of high power lasers for reference beacon projection, control algorithms, and large deformable optics.

EXAMPLE OF APPLICATIONS OF INTEREST TO NOAA

Real-Time Monitoring of Weather

Hurricane/Tornado warnings

- Incorporate Radar Data from multiple systems, i.e. P-3 aircraft, and Unmanned Aerial Vehicles.
- Data sent to other radars or radar cluster array. This can be used to adapt the scanning strategy of the cluster array based on location of tornados.

Tsunami Events

- Tsunami triggers and activates earthquake sensors
- Earthquake sensors trigger Deep Ocean Assessment and Reporting of Tsunamis (DART) & other ship-borne sensors

Water & Air Quality

Water:

Real time measurements of location & concentration of contaminants **PLUS** real time data on tides & currents *yield*

Vital information for containment and warnings

Air:

Air Quality Sensors in affected areas together with

real time numerical model data triggered by

real time sensor event identification provides

emergency managers need to warn public and

stimulates deployment of other sensors.

Items of Interest to NIH

- NIH/NLM
  - Modeling of medical care delivery systems
  - Modeling of physiological processes
  - Dynamic integration of multimedia, multimodal data, created from disparate sources, for a given patient or multiple patients
  - Disaster management medical services
  - …
- NIH/NIGMS
  - Dynamic models of patient response to medical intervention, including drug regiments
  - Dynamic models of metabolic and signaling pathways and networks
  - Models of infectious diseases
  - …

What about Industry & DDDAS

- **Industry has history of**
  - forging new research and technology directions and
  - adapting and productizing technology which has demonstrated promise
- **The present solicitation encourages joint academe/industry research collaborations;**
  - joint projects / early stages
- **However not all projects are expected to have collaborations with industry**
- **Technology transfer**
  - establish path for tech transfer from academic research to industry
  - joint projects, students, sabbaticals (academe <----> industry)
- **Together with Cross-Agency co-ordination, past success stories include: VLSI, Networking, and Parallel and Scalable Computing, etc**
- **Industry is interested in DDDAS**

Impact to CyberInfrastructure

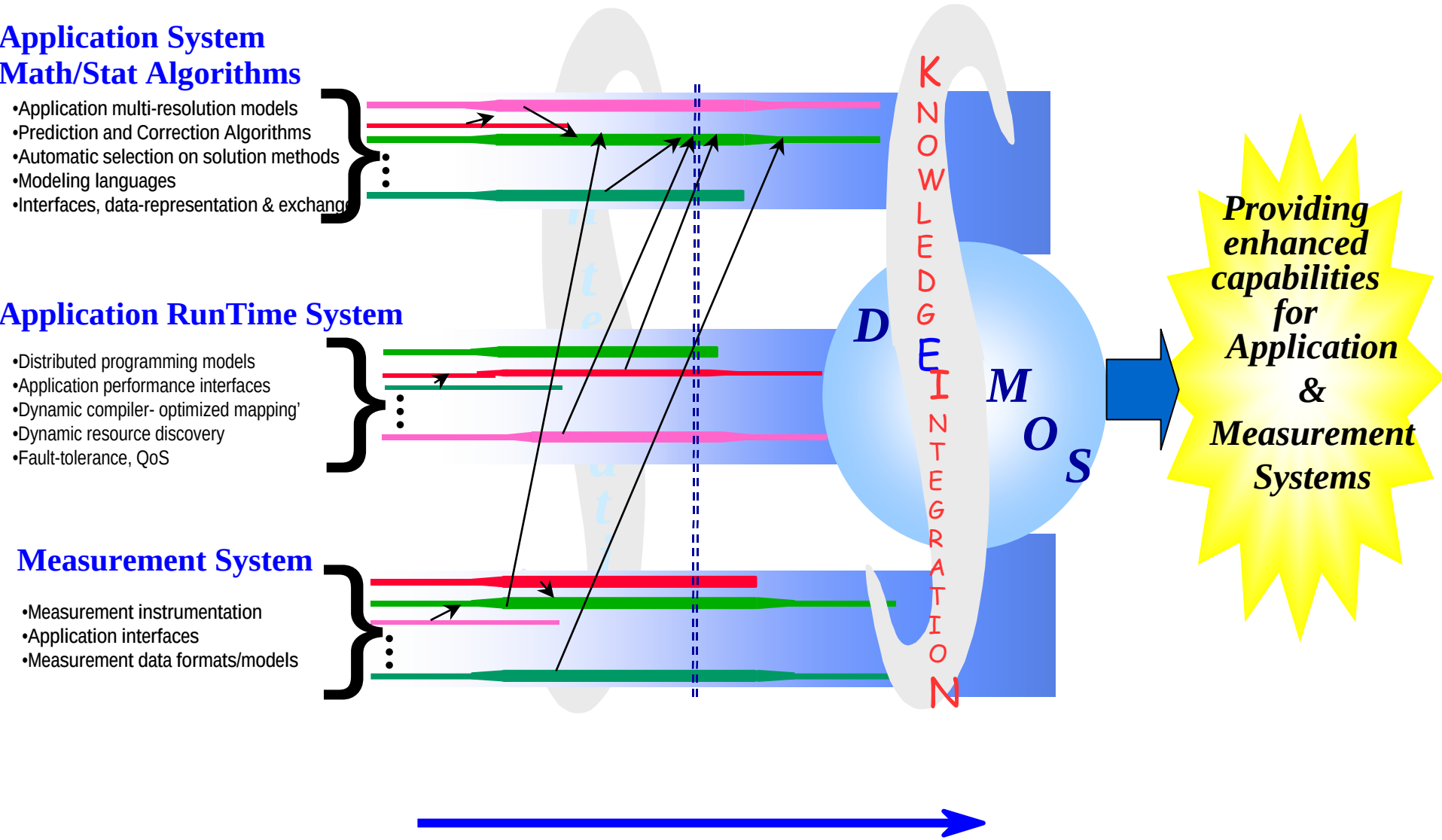
- The CyberInfrastructure that will result when one thinks of the present paradigm of (disjoint) simulations and measurements will be different than the CyberInfrastructure needed to support DDDAS
- DDDAS environments will integrate computational aspects of applications/simulations with experimental infrastructure efforts such as for example NEES, LHC, ChemMatCARS, GEON, NEON, etc…, and enhance the design and deployment of such experimental infrastructures
- In addition systems software support, bandwidth requirements, resource allocation and other middleware and systems software policies, prioritization, security, fault tolerance, recovery, QoS, etc…, will have more stringent requirements when one needs to guarantee data streaming to an executing simulation or control of measurement process (e.g. involving expensive instruments)
- DDDAS will impact the kind of underlying infrastructure that needs to be provided
- Programmatically DDDAS is a research effort

Award Information: Project Categories

- **Three categories of projects:**
  - **Team Multidisciplinary Research Projects (TMRPs)**
    - **3-5 year duration,** each involving 2-5 investigators
    - working collaboratively on application, application measurement and algorithms, and systems software aspects of the projects
  - **Small Multidisciplinary Research Projects (SMRPs)**
    - **3 year duration**, each involving 1-2 investigators,
    - may place emphasis in one or two of the four area components described in this solicitation and
    - must clearly describe advances to be made in the context of enabling DDDAS capability for (a) specified driving application(s).
  - **Small Exploratory Projects (SEPs)**
    - **1 year duration**,
    - to either explore some unusually high-risk ideas, or
    - establish partnerships with researchers in other component areas, or
    - conduct workshops bringing the broader community to articulate specific opportunities

Research and Technology Roadmap

emphasis on multidisciplinary research



Scope of Activities on DDDAS

- We have started seeding DDDAS efforts
  - NSF Workshop on DDDAS, March 2000
  - Primarily through the ITR (Information Technology Research Program FY00-04), in accordance with a major objective of ITR to "fund novel research and spawn new research areas" not funded within existing programs
  - List of DDDAS related projects funded through ITR is in the dddas-webpage: www.cise.nsf.gov
- The present solicitation is intended to broaden the scope of scientific and engineering communities involved in DDDAS research, and fund DDDAS related research in a systematic way
- DDDAS related Workshops (listed in the dddas-webpage)
  - NSF, March 2000
  - International Conf. on Computational Science (ICCS'03)
  - ICCS'04
  - ICCS'05 (May 22-23, 2005)

Award Funding Information for Present Solicitation

- Budget: $15M +…
- Projects must have synergistic multidisciplinary research in:
  - Applications, Math&Stat Algorithms, Systems Software, and Measurement Methods
- Categories of Projects to be supported:
  - SMRP ("small"): up to $600K (total) for 3years
  - TMRP ("team"): up to $2M (total) for 4-5years
  - SEP ("exploratory"): $50K for 1 year
- Projects to be funded:
  - 15-20 in "small" and "team"
  - 10 "exploratory"
- PI Eligibility: an individual can be PI, co-PI or Senior Personnel in only one proposal in this competition

Program Officials Contacts

NSF

- Frederica Darema, Directorate for Computer & Information Science & Engineering
- Mario Rotea, Directorate for Engineering
- Marvin Goldberg, Directorate for Mathematical & Physical Sciences
- Daniel H. Newlon, Directorate for Social, Behavioral & Economic Sciences
- John C. Cherniavsky,, Directorate for Education & Human Resources
- Juan E. Figueroa, SBIR/STTR Programs
- Jeanne E. Hudson, Office of the Director, Office of International Science and Engineering,

NIH

- Charles Friedman, National Library of Medicine, Office of Extramural Programs
- Peter Lyster, National Institute of General Medical Sciences

NOAA

- Robert Bohn, Project Manager, NOAA

EU

- Dr. Kyriakos Baxevanidis, EU e-Infrastructure Program
- Dr. Max Lemke, Grid Research,under the EU Information Society Technologies (IST) Programme

UK

- Dr. James Flemming, e-Sciences RCUK Program

Additional NSF Program Officers involved in this solicitation

- **Directorate for Computer & Information Science & Engineering**
  - Anita LaSalle, Expert, Division of Computer and Network Systems
  - Miriam Heller, Program Director, Division of Shared Cyberinfrastructure
  - Larry Brandt, Program Manager, Division of Information and Intelligent Systems
  - Heasun Park, Program Director, Division of Computing and Communication Foundations
  - Sol Greenspan, Program Director, Division of Computing and Communication Foundations
- **Directorate for Engineering**
  - Ken Chong, Program Director, Division of Civil & Mechanical Systems
  - Jesus de la Garza, Program Director, Division of Civil & Mechanical Systems
  - Suvrajeet Sen, Program Director, Division of Design, Manufacture, & Industrial Innovation
  - Abhijit Deshmukh, Program Director, Division of Design, Manufacture, & Industrial Innovation
  - Bruce Hamilton, Division Director, Division of Bioengineering & Environmental Systems
  - Semahat Demir, Program Director, Division of Bioengineering & Environmental Systems
  - Maria K. Burka, Program Director, Division of Chemical & Transport Systems
  - Triantafillos Mountziaris, Program Director, Division of Chemical & Transport Systems
  - Michael Plesniak, Program Director, Division of Chemical & Transport Systems
  - Radhakisan S. Baheti, Program Director, Division of Electrical & Communications Systems
  - Paul Werbos, Program Director, Division of Electrical & Communications Systems
- **Directorate for Mathematical & Physical Sciences**
  - James Whitmore, Program Director, Division of Physics
  - Brad Keister, Program Director, Division of Physics
  - Guebre Tessema, Program Director (NAF), Division of Materials Research
  - Arthur Ellis, Division Director, Division of Chemistry
  - Nigel Sharp, Program Director, Division of Astronomical Sciences
  - Robert Serfling, Program Director, Division of Mathematical Sciences

DDDAS

Simulations
(Math.Modeling
Phenomenology
Observation Modeling
Design)

Dynamic
Feedback
& Control
Loop

Experiment
Measurements
Field-Data
User

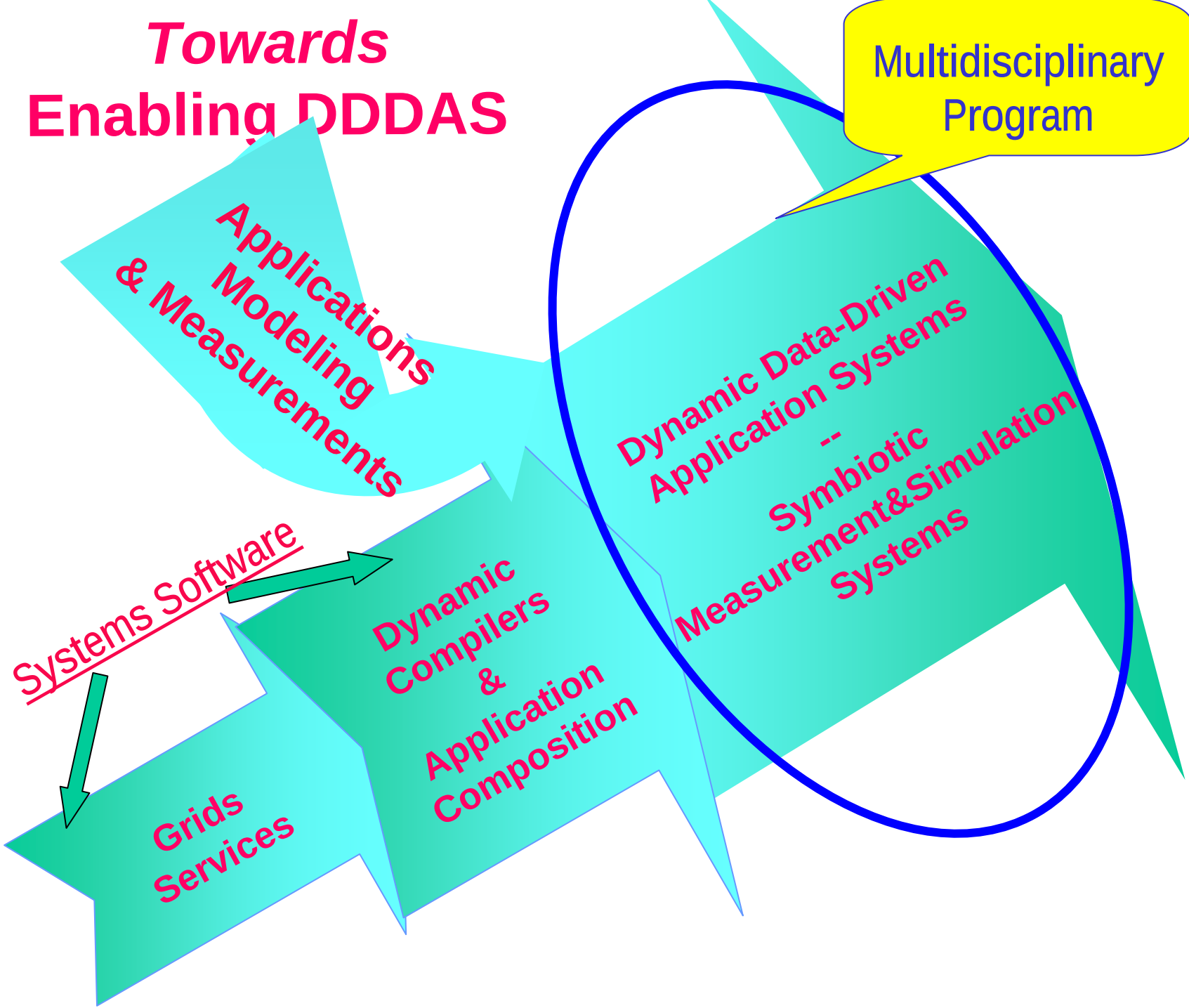
NSF05-570
www.cise.nsf.gov/dddas
Proposal Deadline: June 13, 2005

Enabling the DDDAS vision
rests on
the creativity and resourcefulness
of the research community

DDDAS has potential
for significant impact in
science, engineering, and commercial world,
akin to the transformation effected
since the '50s
by the advent of computers

backup slides

Towards
Enabling DDDAS



NSF March 2000 Workshop on DDDAS

(Co-Chairs: Craig Douglas, UKy; Abhi Desmukh, UMass)

Invited Presentations

- New Directions on Model-Based Data Assimilation (Chemical Appl's)
  Greg McRae, Professor, MIT
- Coupled atmosphere-wildfire modeling
  Janice Coen, Scientist, NCAR
- Data/Analysis Challenges in the Electronic Commerce Environment
  Howard Frank, Dean, Business School, UMD
- Steered computing - A powerful new tool for molecular biology
  Klaus Schulten, Professor, UIUC, Beckman Institute
- Interactive Control of Large-Scale Simulations
  Dick Ewing, Professor, Texas A&M University
- Interactive Simulation and Visualization in Medicine: Applications to Cardiology, Neuroscience and Medical Imaging
  Chris Johnson, Professor, University of Utah
- Injecting Simulations into Real Life
  Anita Jones, Professor, UVA

Workshop Report: www.cise.nsf.gov/dddas

DDDAS Funding Opportunities

NSF

- NGS: The Next Generation Software Program (1998-)
  - develops systems software supporting dynamic resource execution
- Scalable Enterprise Systems Program (1999, 2000-2003)
  - geared towards "commercial" applications
- ITR: Information Technology Research (NSF-wide, FY00-04)
  - has been used as an opportunity to support DDDAS related efforts
  - in FY00, 1 NGS/DDDAS proposal received; deemed best, funded
  - in FY01, 46 ~DDDAS pre-proposals; 24 proposals; 8 awarded
  - in FY02, 31 ~DDDAS proposals; 8(10) awards
  - in FY03, 35- "small" , 38-"medium" , 3-"large" ; awarded 8
  - in FY04: ~100 small-medium; awarded: 10
- DDDAS program in FY05
  - multiple NSF Directorates, other agencies (NIH, NOAA, …), including NSF SBIR/STTR and International Programs
  - Cooperating with EU Grids and e-Sciences Program

"~DDDAS" proposals awarded in FY00 ITR Competition

- **Pingali, Adaptive Software for Field-Driven Simulations**

"~DDDAS" proposals awarded in FY01 ITR Competition

- Biegler – Real-Time Optimization for Data Assimilation and Control of Large Scale Dynamic Simulations
- Car – Novel Scalable Simulation Techniques for Chemistry, Materials Science and Biology
- Knight – Data Driven design Optimization in Engineering Using Concurrent Integrated Experiment and Simulation
- Lonsdale – The Low Frequency Array (LOFAR) – A Digital Radio Telescope
- McLaughlin – An Ensemble Approach for Data Assimilation in the Earth Sciences
- Patrikalakis – Poseidon – Rapid Real-Time Interdisciplinary Ocean Forecasting: Adaptive Sampling and Adaptive Modeling in a Distributed Environment
- Pierrehumbert- Flexible Environments for Grand-Challenge Climate Simulation
- Wheeler- Data Intense Challenge: The Instrumented Oil Field of the Future

"~DDDAS" proposals awarded in FY02 ITR Competition

- Carmichael – Development of a general Computational Framework for the Optimal Integration of Atmospheric Chemical Transport Models and Measurements Using Adjoints
- Douglas-Ewing-Johnson – Predictive Contaminant Tracking Using Dynamic Data Driven Application Simulation (DDDAS) Techniques
- Evans – A Framework for Environment-Aware Massively Distributed Computing
- Farhat – A Data Driven Environment for Multi-physics Applications
- Guibas – Representations and Algorithms for Deformable Objects
- Karniadakis – Generalized Polynomial Chaos: Parallel Algorithms for Modeling and Propagating Uncertainty in Physical and Biological Systems
- Oden – Computational Infrastructure for Reliable Computer Simulations
- Trafalis – A Real Time Mining of Integrated Weather Data

"~DDDAS" proposals awarded in FY03 ITR Competition

- Baden – Asynchronous Execution for Scalable Simulation in Cell Physiology
- Chaturvedi– Synthetic Environment for Continuous Experimentation (Crisis Management Applications)
- Droegemeier-Linked Environments for Atmospheric Discovery (LEADS)
- Kumar – Data Mining and Exploration Middleware for Grid and Distributed Computing
- Machiraju – A Framework for Discovery, Exploration and Analysis of Evolutionary Data (DEAS)
- Mandel – DDDAS: Data Dynamic Simulation for Disaster Management (Fire Propagation)
- Metaxas- Stochastic Multicue Tracking of Objects with Many Degrees of Freedom
- Sameh – Building Structural Integrity
- {Sensors Program: Seltzer – Hourglass: An Infrastructure for Sensor Networks}

"~DDDAS" proposals awarded in FY04 ITR Competition

- Brogan – Simulation Transformation for Dynamic, Data-Driven Application Systems (DDDAS)
- Baldridge – A Novel Grid Architecture Integrating Real-Time Data and Intervention During Image Guided Therapy
- Floudas-In Silico De Novo Protein Design: A Dynamically Data Driven, (DDDAS), Computational and Experimental Framework
- Grimshaw: Dependable Grids
- Laidlaw: Computational simulation, modeling, and visualization for understanding unsteady bioflows
- Metaxas – DDDAS - Advances in recognition and interpretation of human motion: An Integrated Approach to ASL Recognition
- Wheeler: Data Driven Simulation of the Subsurface: Optimization and Uncertainty Estimation

DDDAS Workshops

- NSF Workshop, March 2000
- DDDAS Workshop, ICCS'03
- DDDAS Workshop, ICCS'04
- DDDAS Workshop, (May22-23) ICCS'05

Tally Points

- ITR Program was initiated to start new research, not previously funded by existing NSF programs
- ITR was used to spawn a significant number on ~DDDAS projects
- majority of funds for DDDAS from ITR - additional funding sources for other NSF Programs: NGS, SES, Sensors, BITS, etc
- About 40 projects
- Project sizes: $400K-$12M, majority $1-3M, one: $12M
- ITR funds on DDDAS: ~$60M (cumulative)

Why Now is the Time for DDDAS

- Technological progress has prompted advances in some of the challenges
  - Computing speeds advances: uni- and multi-processor systems, High-Performance Systems, Grid Computing, Sensor Networks
  - Systems Software
  - Applications Advances (parallel & grid computing)
  - Algorithms advances (e.g.: parallel &grid computing, numeric and non-numeric techniques: adaptive, asynchronous algorithms, dynamic meshing, data assimilation, 3DVAR/4DVAR, chaotic Monte-Carlo)
- The talk will provide examples of efforts in:
  - Applications, Algorithms, Instrumentation, Systems Software

Procedural Logistics on this Webcast

- Presentations on the Program, followed by Q&A
- Qs have been submitted by email a priori
- First will address Qs from in-person present
- Then Qs submitted a priori
- Additional Qs may be submitted during this presentation, and they will be addressed subsequently on an FCFS basis
- Qs not addressed due to time constraints: the responses will be posted in the FAQ section of the dddas webpage: www.cise.nsf.gov/dddas